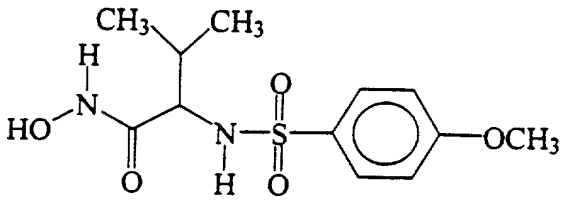
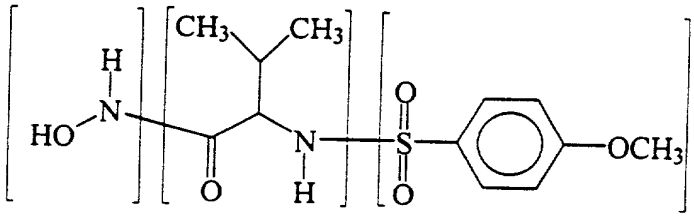
Compound CI



$C_{12}H_{18}N_2O_5S$



	F_i	F_{ii}	F_{iii}
Molecular formula	H_2NO	C_5H_9NO	$C_7H_7O_3S$

Figure 1

Addition of fragments to yield compounds

Table

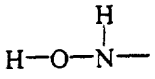
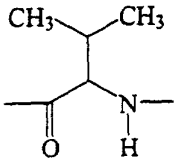
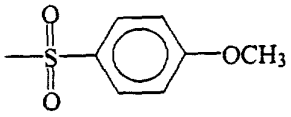
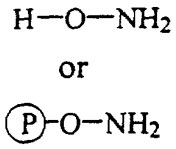
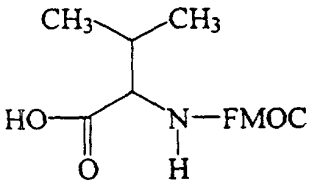
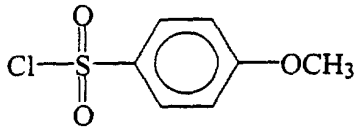
Fragment Identifier	Structure	Name	Molecular formula	Other
F_i		Hydroxylamine	H_2NO	...
F_{ii}		Amino acid	C_5H_9NO	...
F_{iii}		Sulfonyl	$C_7H_7O_3S$	...

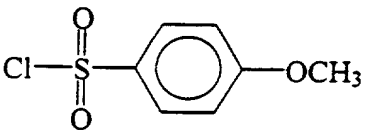
Figure 2

Reagents	Identifier	Name	Properties
	R_i	Hydroxylamine	...
	R_{ii}	FMOC blocked amino acid	...
	R_{iii}	Sulfonylchloride	...

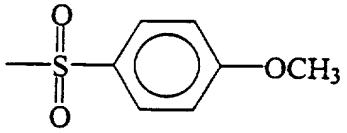
Ⓟ = Solid support

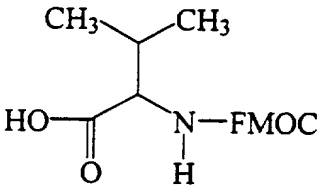
Figure 3

Transformation

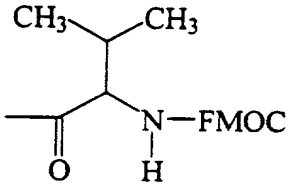
T_i  Reagent R_i

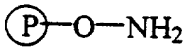
reaction conditions alpha

 Fragment F_i

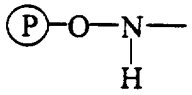
T_{ii}  Reagent R_{ii}

reaction conditions beta

 Fragment F_{ii}

T_{iii}  Reagent R_{iii}

reaction conditions gamma

 Fragment F_{iii}

Ⓟ = Solid support

Figure 4

Common Fragment / Different Reagents and Transformations

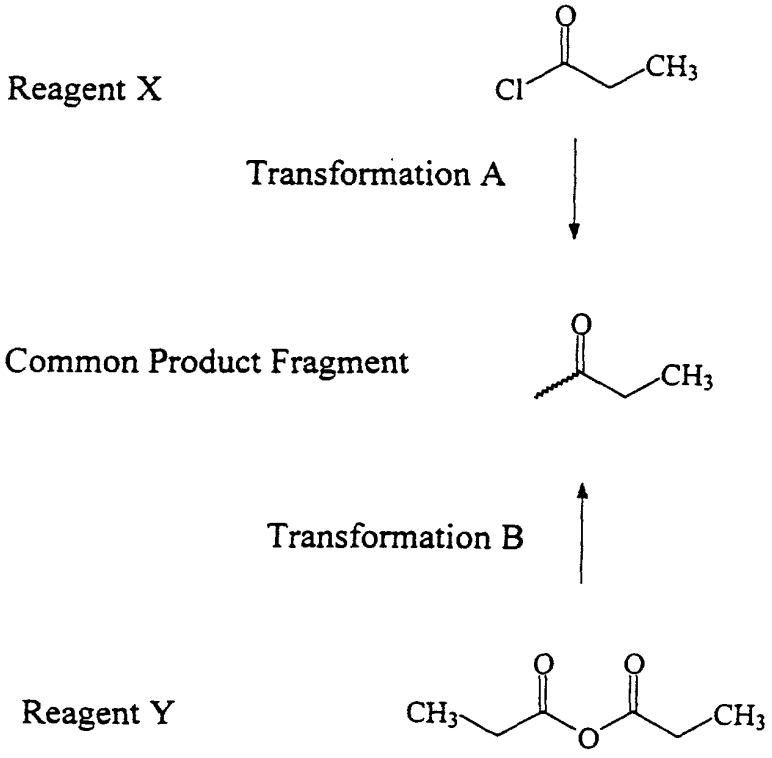


Figure 5

Common Fragment / Different Reagents and Transformations

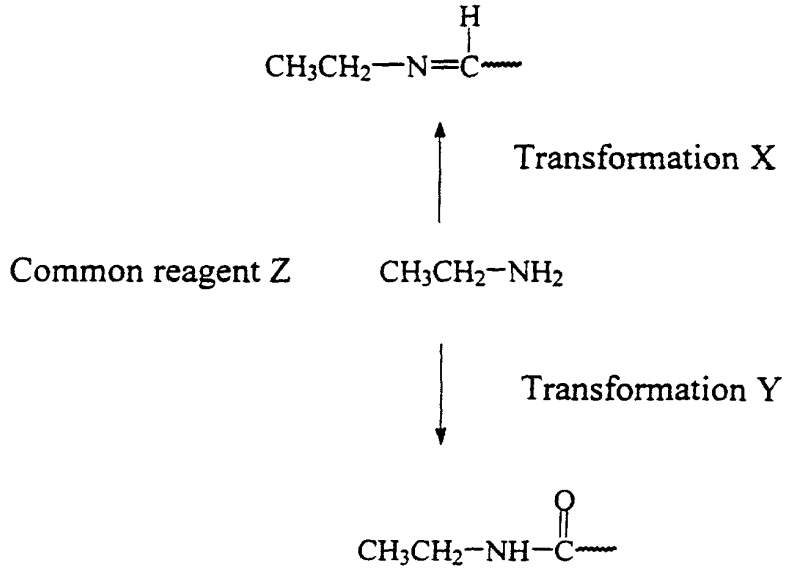


Figure 6a

Common Reagent

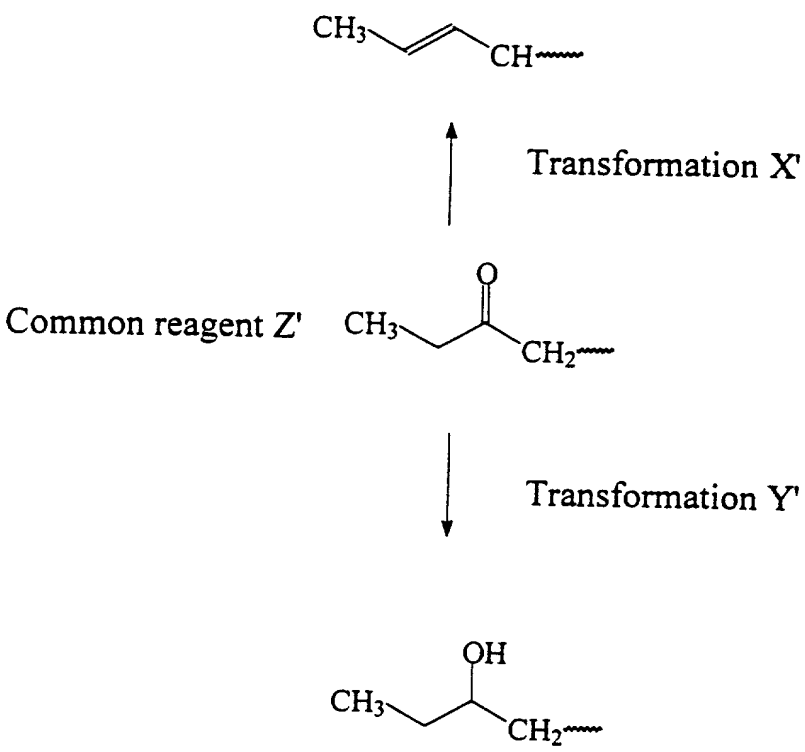
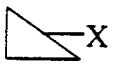
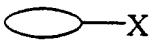
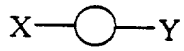
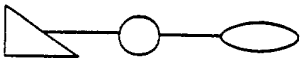


Figure 6b

Symbolic addition of fragments to yield compound

Symbolic Structure	Symbolic Identifier	Molecular formula
Fragment		
	$F_{i'}$	$C_uH_vN_w$ ...
	$F_{ii'}$	$C_uH_vN_w$ ...
	$F_{iii'}$	$C_uH_vN_w$ ...
Compound		
	CI'	$C_uH_vN_w$ ...

$$\text{Molecular formula } F_{i'} + \text{Molecular formula } F_{ii'} + \text{Molecular formula } F_{iii'} = \text{Molecular formula } CI'$$

Figure 7

Symbolic Reagent Table

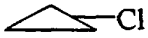
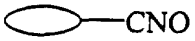
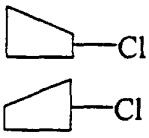
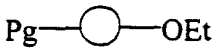
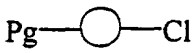
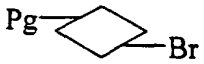
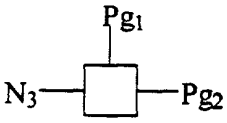
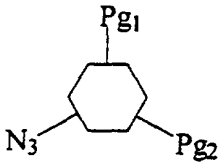
Identifier	Name	Structure	Molecular formula
R1	xxx		xxx
R2	...		...
R3	...		...
R4	...		...
R5	...		...
R6	...		...
R7	...		...
R8	...		...
R9	...		...
R10	...		...

Figure 8

Symbolic Fragment Table

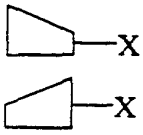
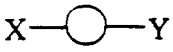
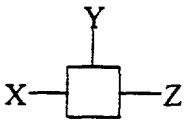
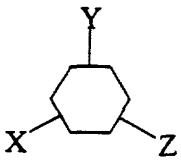
Identifier	Symbolic Structure	Molecular formula	Molecular Weight
F1		xxx	xxx
F2		...	...
F3		...	...
F4		...	...
F5		...	...
F6		...	...
F7		...	...
F8		...	...

Figure 9

Symbolic Transformation Table

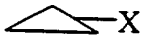
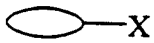
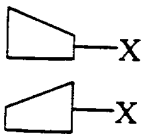
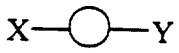
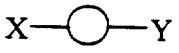
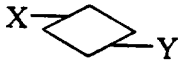
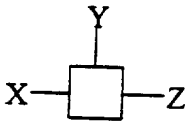
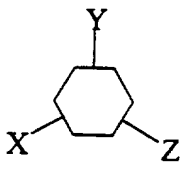
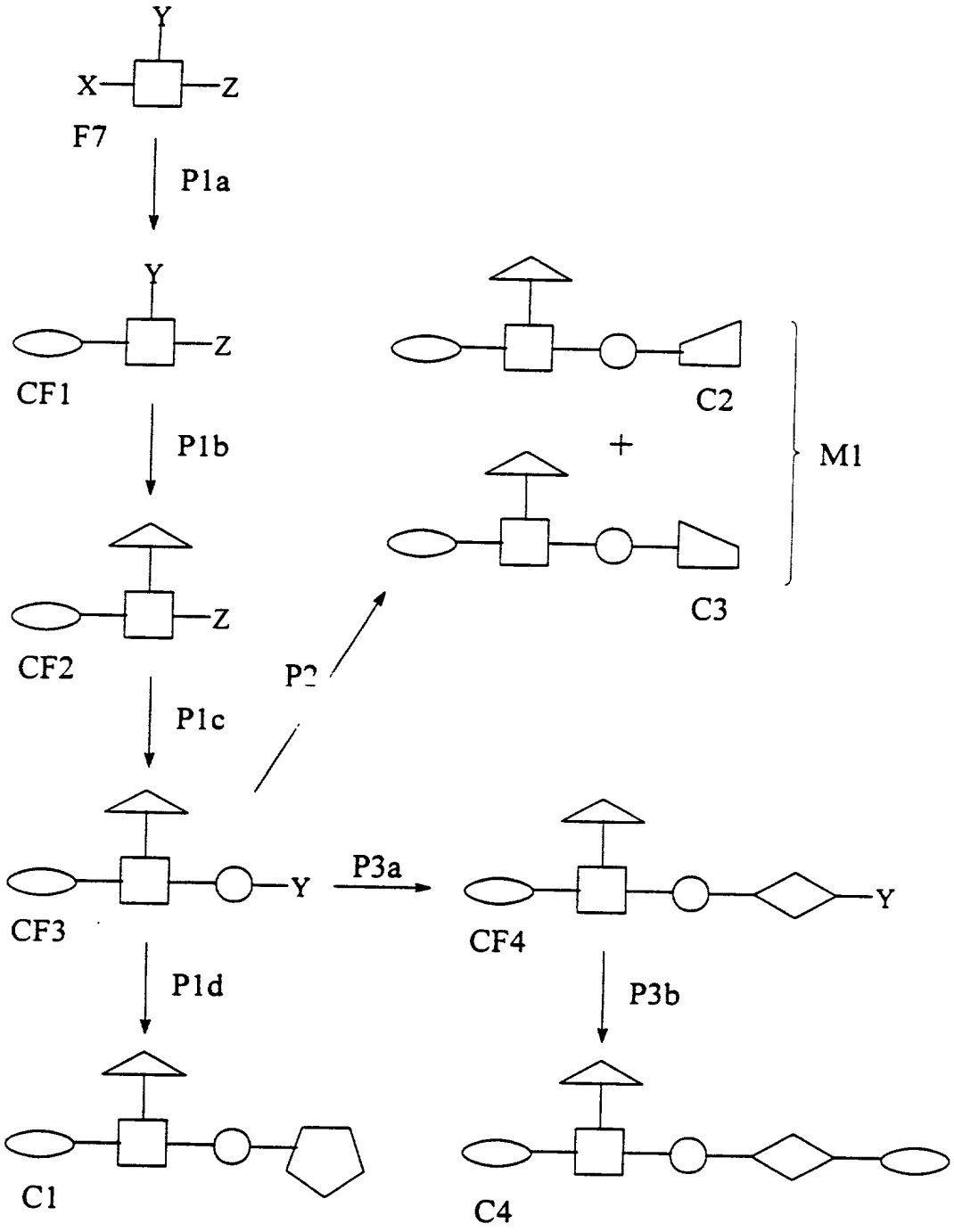
Identifier		Symbolic Reactions		Reagent
T1	F1		R1	conditions α
T2	F2		R2	conditions β
T3	F3		R3	conditions α
T4	F3		R4	conditions α
T5	F4		R5	conditions α
T6	F5		R6	conditions ε
T7	F5		R7	conditions α
T8	F6		R8	conditions α
T9	F7		R9	conditions γ
T10	F8		R10	conditions γ

Figure 10

Single Compounds and Mixtures



P = synthetic path
F = fragment
C = compound
CF = complex fragment
M = mixture

Figure 11

Mixture 2

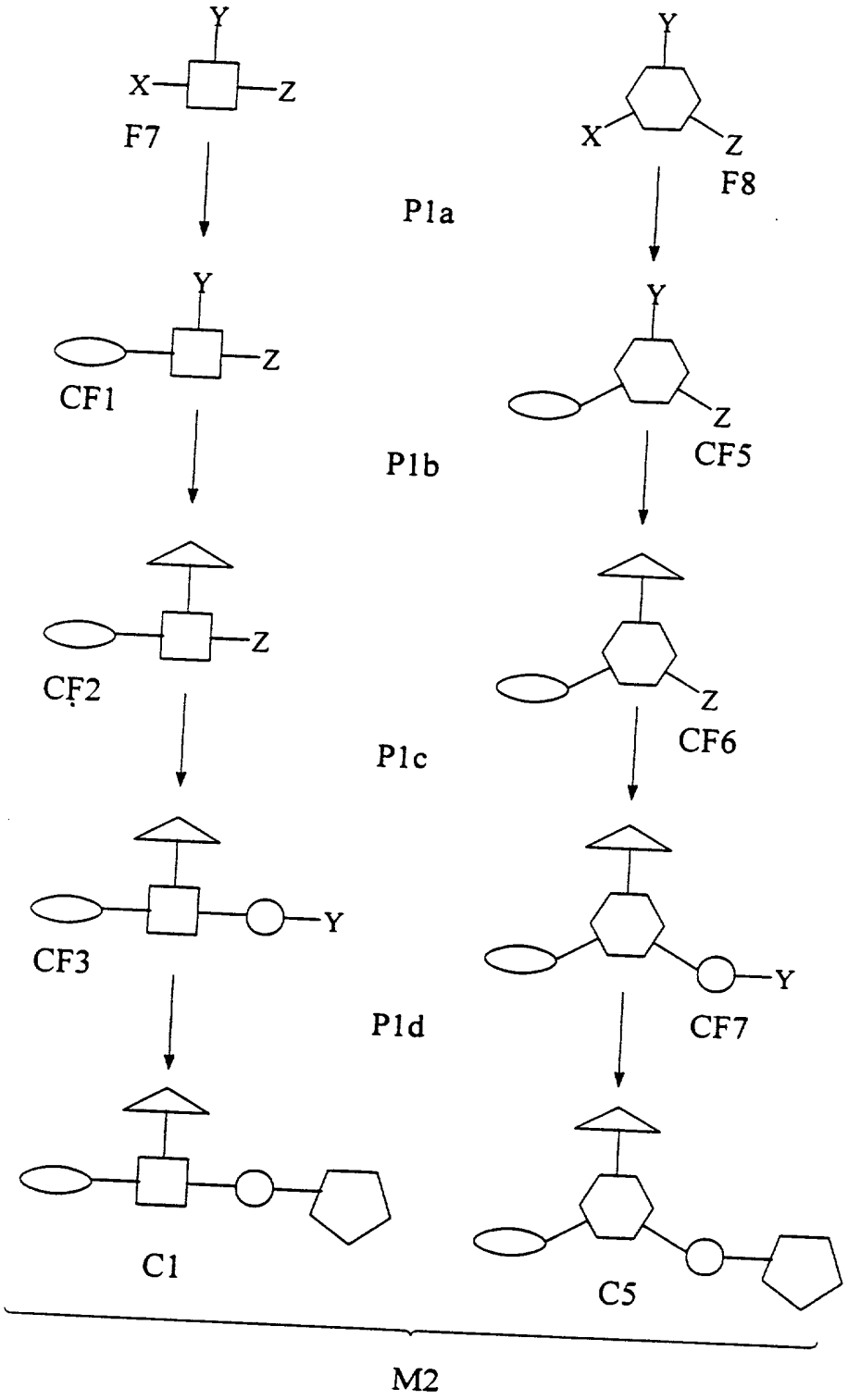


Figure 12

Mixture 3

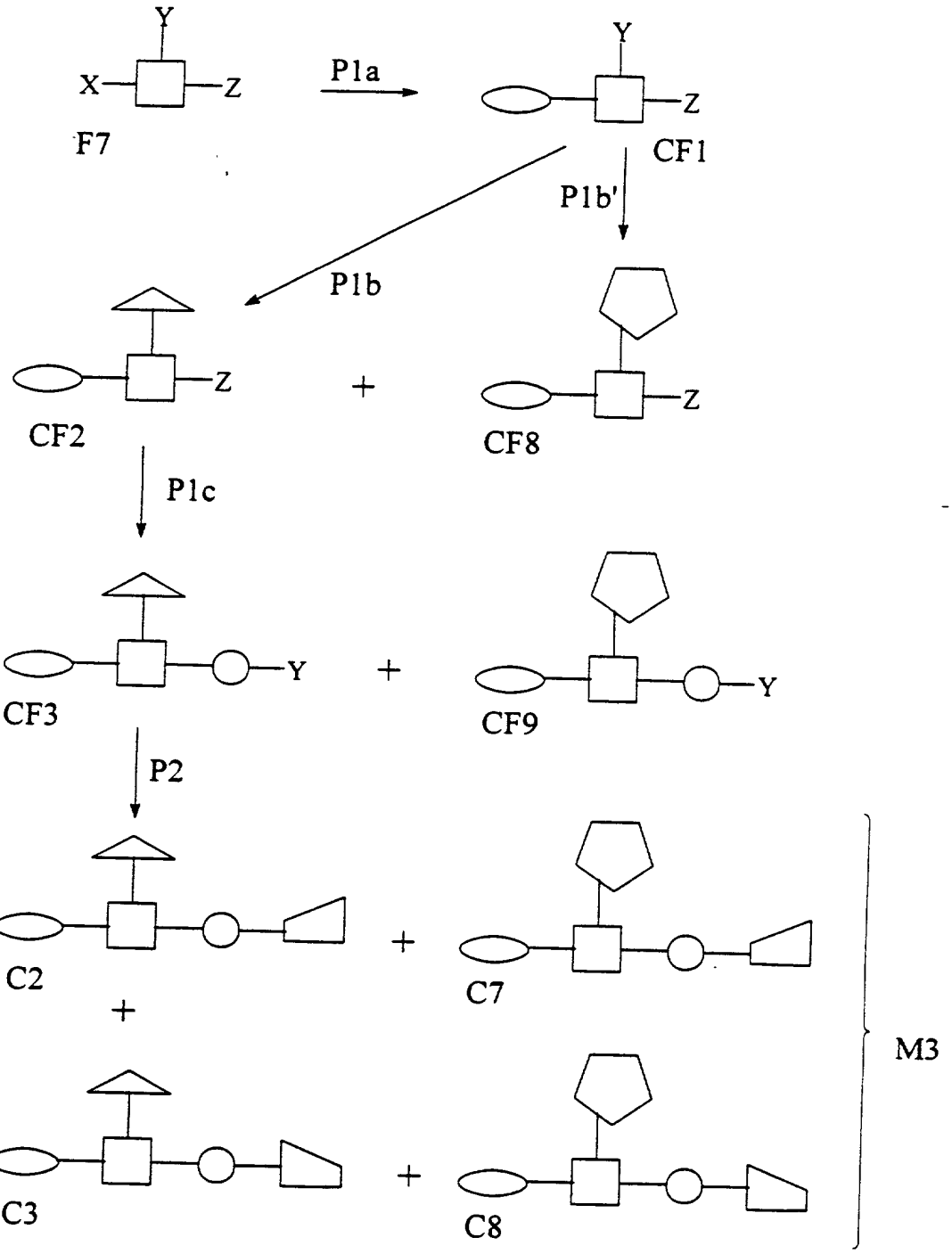
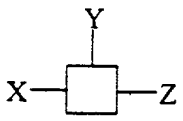


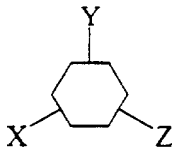
Figure 13

Mixture 4

2 Starting Fragments

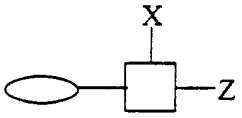


F7

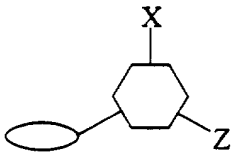


F8

2 Complex Fragments

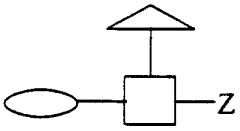


CF1

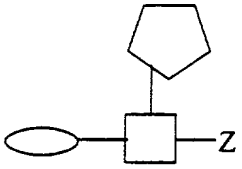


CF5

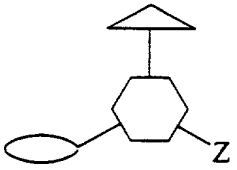
4 Complex Fragments



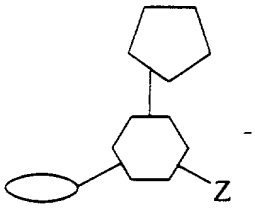
CF2



CF8

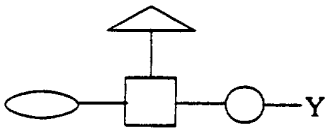


CF 6

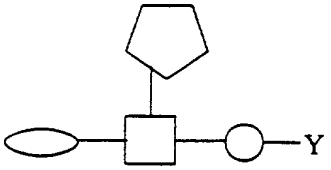


CF11

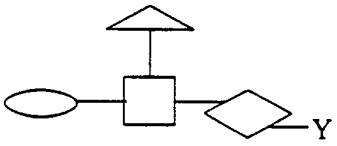
8 Complex Fragments



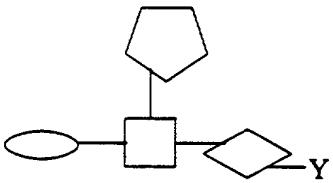
CF3



CF9



CF12



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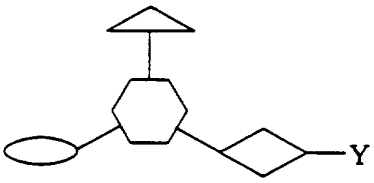
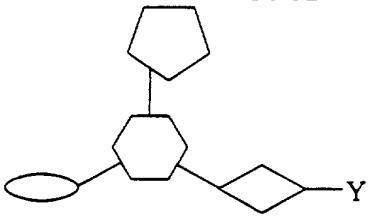
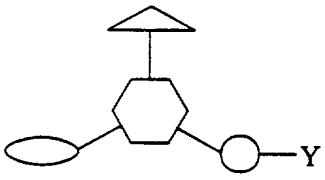


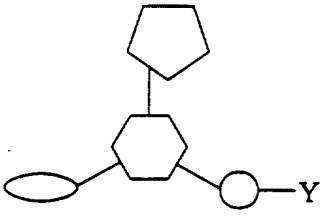
CF15



CF16



CF 7



CF14

Figure 14a

Mixture 4 (continued)

16 compounds

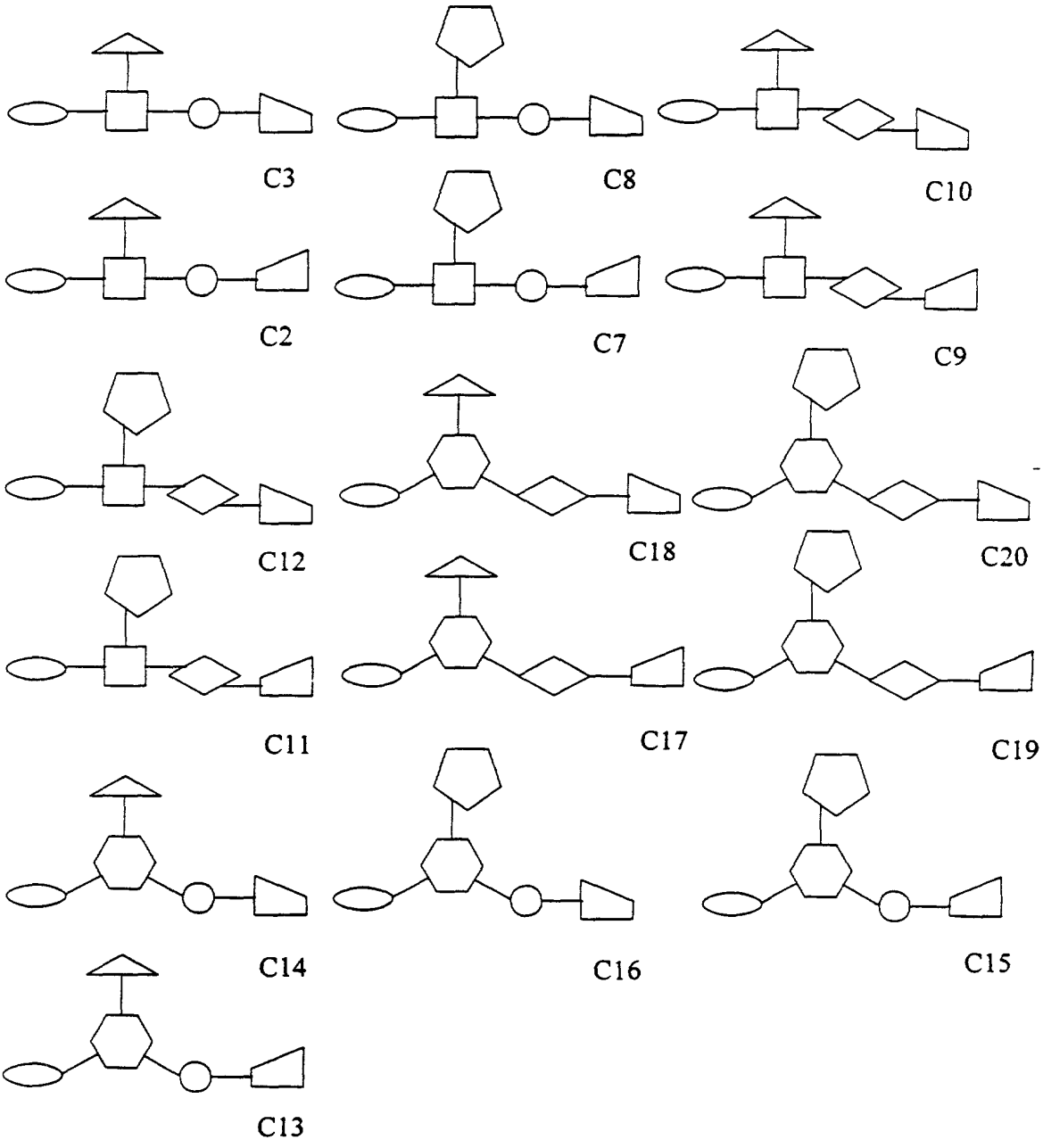


Figure 14b

Tracking Table for Compound C1

(a) By Fragments:

n	n+1	n+2
F7	F2 F1 F5	F3

(b) By Transformations:

Synthesis Path 1

n	n+1	n+2
T9	T2 T1 T6	T3

Synthesis Path 2

n	n+1	n+2
T9	T2 T1 T7	T3

Synthesis Path 3

n	n+1	n+2
T9	T2 T1 T6	T4

Synthesis Path 4

n	n+1	n+2
T9	T2 T1 T7	T4

Figure 15

Tracking Table

Tracking M1

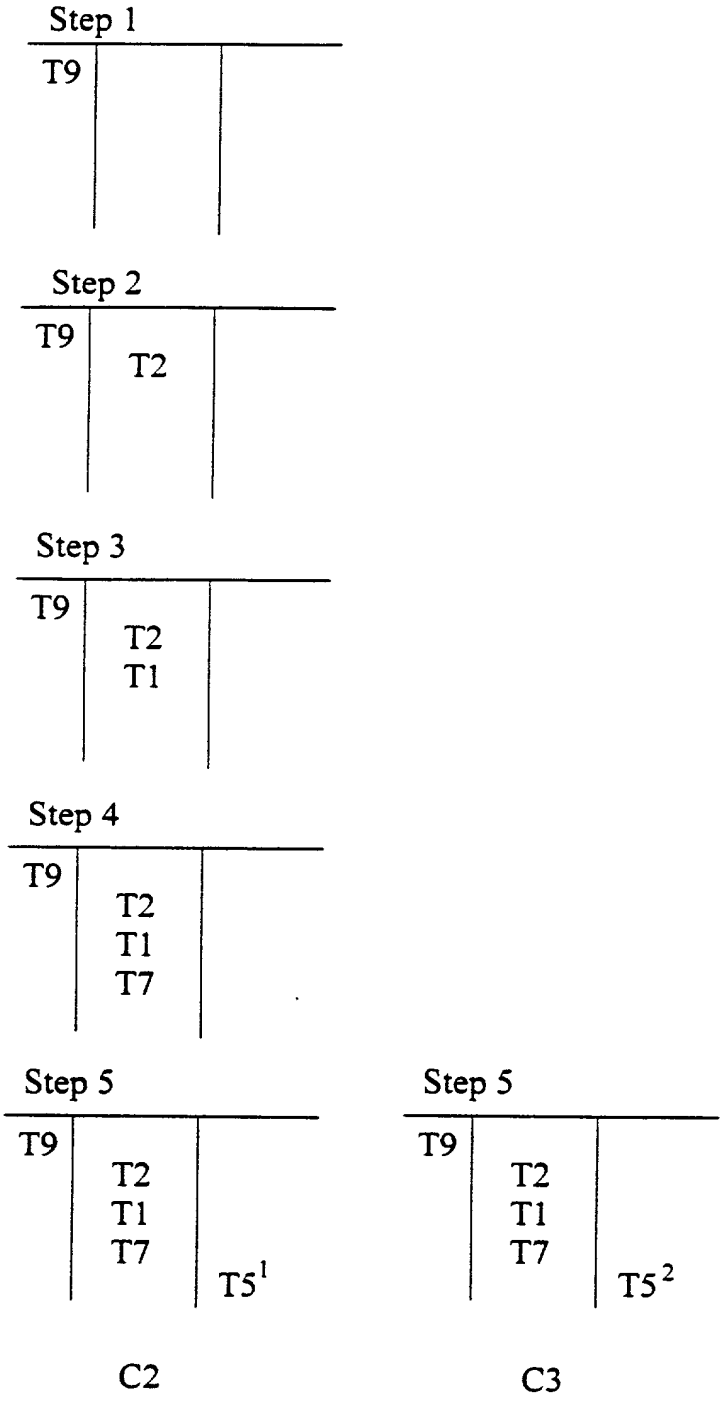
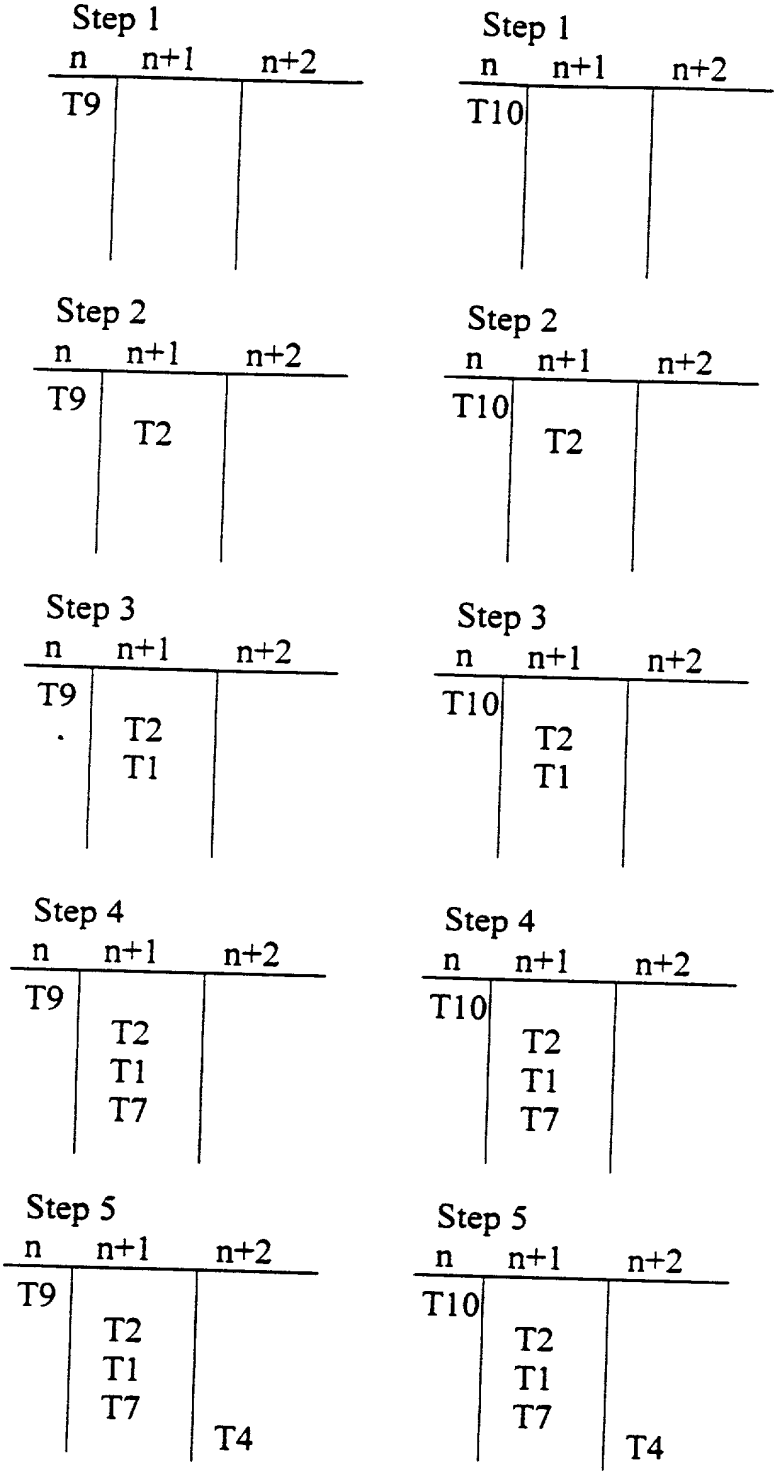


Figure 16

Tracking Table

Tracking M2



C1

C5

Figure 17

Tracking Table

Tracking M3

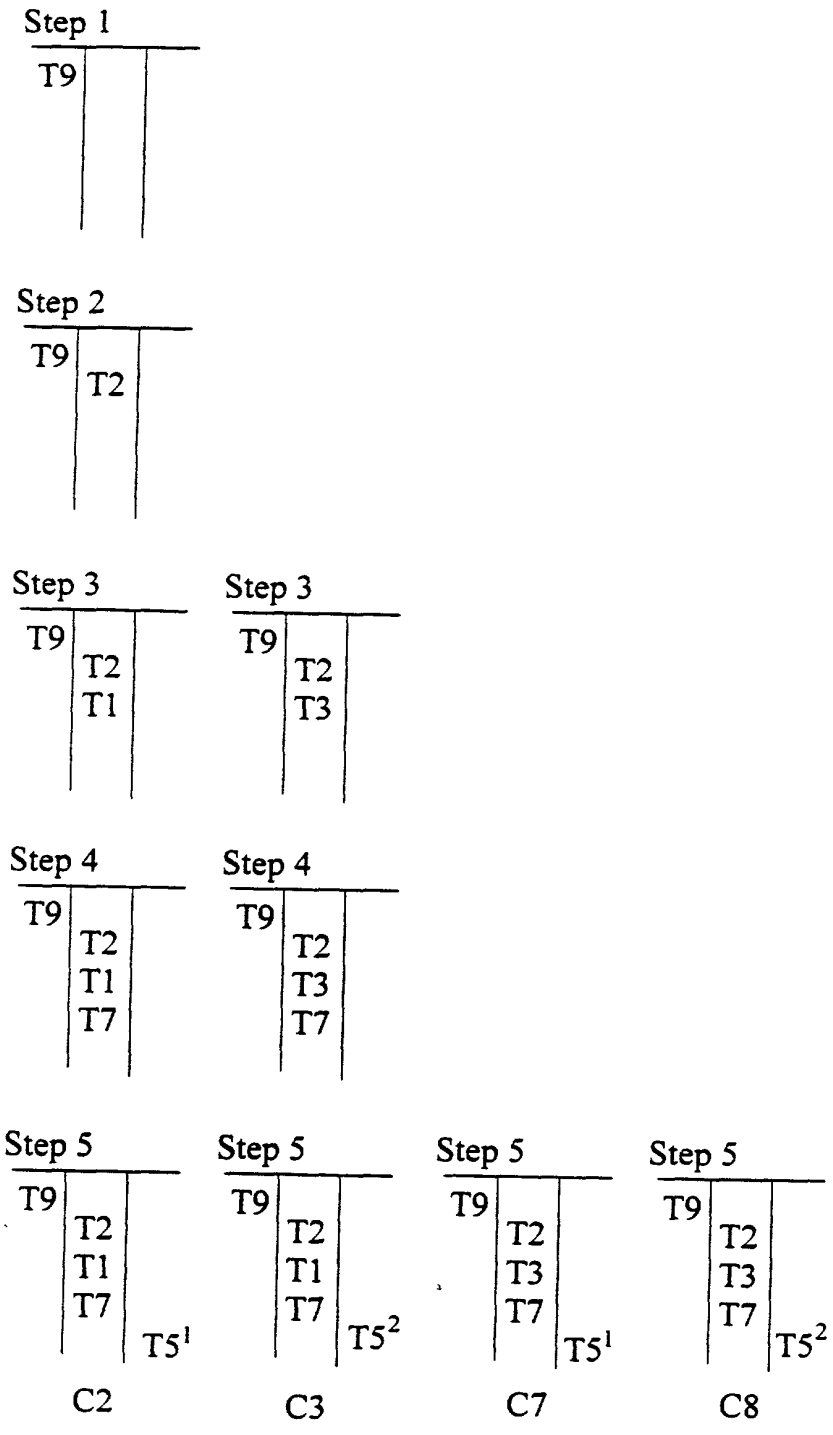


Figure 18